TRUCHAS Installation Guide

Neil Carlson

Version 2.6.0
April 12, 2012

LA-UR-12-20536

LA-UR-12-20536

TRUCHAS is a relatively portable code and is not especially particular about what platform it runs on. It requires a good Fortran compiler that correctly implements the Fortran 95 standard. Surprisingly, this has been perhaps the biggest challenge in porting to a new platform. TRUCHAS has been run on a wide variety of unix-like platforms, many of which no longer exist. Usage in recent years has been almost exclusively on x86-64 architecture, 64-bit Linux platforms, both individual workstations and large, high-performance clusters. It is also known to run on OS X 10.5 (Intel). The TRUCHAS developers currently test and run on platforms with the following features:

- Intel/AMD x86-64
- 64-bit Linux: Red Hat Enterprise Linux 4 and 5; Fedora 14, 15, 16; Ubuntu is reported to work also.
- Fortran compilers: NAG version 5.2, 5.3; Pathscale version 3.1, 3.2; G95 (32-bit default integer version from 8/2010; http://www.g95.org). Compilers which have *not* worked in the past include Intel, PGI, and gfortran.
- Open MPI 1.4 and 1.5.

1 Obtaining the Distribution

The normal distribution mechanism for TRUCHAS is through the Telluride website at

http://telluride.lanl.gov

To obtain access to the TRUCHAS download page you need an upgraded account. If you do not already have one, you may create a basic account by clicking on the **New user?** link on the left of the main page. Then follow the directions on the **contact info** page to have your account upgraded. This last step requires human intervention and may take several days. Once you are logged into the website with an upgraded account, the **downloads** page becomes visible. If necessary, the distribution can be provided on a CD; send a request to telluride-support@lanl.gov.

2 Prerequisites

TRUCHAS relies on a number of third party packages. Some are included in the distribution and automatically built as part of the TRUCHAS build, and most of the others are available as standard OS binary packages, at least for the most popular Linux distributions. There's likely only one third party package that needs to be installed prior to building TRUCHAS.

LA-UR-12-20536

2.1 Standard OS Packages

The following external packages may already exist on your system, and if not, may be available as standard binary OS packages. This is true for the most popular Linux distributions.

2.1.1 Python and NumPy

TRUCHAS uses Python to parse and post-process the TRUCHAS output files and to run the regression suite. Versions 2.5 through 2.7 should work. The Python package NumPy (http://www.numpy.org) is a required add-on to your Python installation. Version 1.4 is known to work. Version 1.5 mostly works and is probably adequate, but version 1.6 does not work with TRUCHAS at all. To see if it is present and verify the version, start an interactive python session and import the numpy module:

```
% python
Python 2.7.2 (default, Oct 27 2011, 01:40:22)
[GCC 4.6.1 20111003 (Red Hat 4.6.1-10)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
>>> numpy.__version__
'1.4.1'
```

If importing numpy results in an error message, it will need to be installed. First check whether an official NumPy package exists for your OS. If not, see the link above for obtaining the package and simple instructions for installing it. Note the required version.

2.1.2 MPI

If you intend to build a parallel version of TRUCHAS you need an implementation of MPI. The TRUCHAS developers currently use Open MPI v1.4, but other implementations like MPICH2 should work as well. Note that TRUCHAS only uses the C language MPI bindings.

2.2 Hypre

Hypre is a library of high performance preconditioners that features parallel multigrid methods for both structured and unstructured grid problems. It is developed by the Center for Applied Scientific Computing (CASC) at Lawrence Livermore National Laboratory.

The source distribution for the hypre library can be obtained from

http://computation.llnl.gov/casc/hypre/software.html

TRUCHAS currently requires version 2.6.0b.

After unpacking the hypre distribution, it must be configured and built using the same compilers that will be used to build TRUCHAS. Two versions of the library can be built. The serial TRUCHAS build will require the serial library, and the parallel TRUCHAS build will require the parallel library. Build the version you need (or both).

Note that TRUCHAS only uses the C language bindings of the hypre library; to prevent the Fortran bindings from being built, set the environment variable `F77` to the empty string `""` before running the configure script.

When building both versions of the library, it is recommended to start from scratch when building the second version by completely removing the hypre source tree after installing the the first version, and unpacking a fresh copy of the hypre source tree. This avoids any lingering files from the first build interferring with the second.

2.3 Installing the serial hypre library

Change into the `src` directory of the hypre source tree and run the following commands to configure, build, and install the library. The configure script looks for a C and C++ compiler in your path; you can manually specify the compilers by setting the `CC` and `CXX` environment variables to the desired compiler paths prior to running the configure script.

```
./configure --prefix=/usr/local/hypre-2.6.0b/serial \
            --without-fei --without-MPI
make
make install
```

Replace the value of the `--prefix` option with the directory where you want the serial library and header files installed. You will need write permission on that directory. Note the name of the directory; the library will be installed in the `lib` subdirectory and the environment variable `HYPRE_SERIAL_LIB_DIR` will need to be set to the full path of that subdirectory when building TRUCHAS.

2.4 Installing the parallel hypre library

Change into the `src` directory of the hypre source tree and run the following commands to configure, build, and install the library. The configure script looks for MPI C and C++ compiler wrappers in your path (e.g., `mpicc` and `mpiCC`); you can manually specify the compilers by setting the `CC` and `CXX` environment variables to the desired compiler paths prior to running the configure script.

```
./configure --prefix=/usr/local/hypre-2.6.0b/parallel \
            --without-fei
make
make install
```

Replace the value of the `--prefix` option with the directory where you want the parallel library and header files installed. You will need write permission on that directory. Note the name of the directory; the library will be installed in the `lib` subdirectory and the environment variable `HYPRE_PARALLEL_LIB_DIR` will need to be set to the full path of that subdirectory when building TRUCHAS.

This assumes your MPI installation provides the MPI compiler wrappers. If not, you will need to manually specify the normal C and C++ compilers using the `CC` and `CXX` environment variables, and supply the configure script with the paths to the MPI include and library directories using its `--with-MPI-include` and `--with-MPI-lib-dirs` options.

2.5 Included Packages

For reference, the following external packages are included in the TRUCHAS distribution:

- Chaco version 2.2, from Sandia National Laboratories (LGPL license), is used to compute a parallel decomposition of the mesh.
- Chaparral version 3.2, from Sandia National Laboratories (LGPL license), is used to compute radiation view factors used by the enclosure radiation model.
- NetCDF version 4.1.3, from `http://www.unidata.ucar.edu` (MIT-style license), is used to read and write netCDF files. This version is patched with the so-called "large model modifications" required by ExodusII-format mesh files.

These packages are automatically built as part of the TRUCHAS build. Should something unexpected happen, however, they can be found in the `truchas/packages` directory.

3 Building TRUCHAS

After ensuring the prerequisites are satisfied, you are ready to build TRUCHAS. Begin by unpacking the gzip-compressed tar archive of the distribution. This will create a directory named `truchas-x.y.z`, where `x.y.z` is the current version number. Change into that directory.

Set your environment variables `HYPRE_SERIAL_LIB_DIR` and `HYPRE_PARALLEL_LIB_DIR` to the directories containing the hypre libraries as described in Section 2.3 and Section 2.4.

If you are building a parallel TRUCHAS version, you will need to edit the `src/options/libraries` file and set the variables `MPI_INCLUDE_DIR`, `MPI_LIB_DIRS`, and `MPI_LIBS` to the appropriate values for your MPI installation. The file contains examples to guide you. Your MPI C compiler wrapper may also have an option that will show you this information; for example with Open MPI, `mpicc -showme`.

The TRUCHAS executable is built with a make command of the form

```
make compiler=<compiler> <target>
```

where `<compiler>` specifies the Fortran compiler and `<target>` specifies the version of TRUCHAS executable to build. The possible `<compiler>` values are `pathscale`, `nag`, or `g95`. The possible `<target>` values are

```
all-serial-debug
all-parallel-debug
all-serial-opt
all-parallel-opt
```

which specify debug/optimized versions of a serial/parallel TRUCHAS. If all goes well, you will find the executable in the `bin` directory.

3.1 Testing the Executable

You may test your TRUCHAS executable by running the test suite. For example, if you built an optimized serial executable using g95, you would run the test suite with

```
make compiler=g95 test-serial-opt
```

Each test will report either pass or fail.

3.2 Some Build Details

When things go wrong with the TRUCHAS build it is helpful to have a better understanding of the process. The TRUCHAS build proceeds in several stages.

- First, each of the packages in the `packages` directory are built within their own directories.
- Next the TRUCHAS code is built. Its sources are found in the `src` directory, but all the build files are located in a subdirectory of the `build` directory.
- Finally the TRUCHAS output parser tool is built

The `src/options` directory contains the make configuration files. In particular, in contains a number of `cf.*` files that define the make configuration for specific platforms (operating system, hardware architecture, compiler, etc.) This is the place to start when porting to a new platform.

4 Problems

Please report any problems installing or running TRUCHAS to telluride-support@lanl.gov. Please include details about your platform and any other information needed to identify the problem.